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XAS studies on $HfO_2/SiO_2/Si$ gate stacks for CMOS applications

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The continuous scaling of semiconductor devices to achieve higher speed, density and computational ability, at lower power consumption and cost has been maintained for more than 30 years. One critical component, the gate dielectric, is now less than 2nm thick in state-of-the-art CMOS devices, but can not be indefinitely scaled down with current materials. Thermally grown SiO_2 is currently the material of choice for gate dielectrics however it is reaching its fundamental limits primarily due to high leakage currents across the dielectric.

HfO_2 is one of the alternative gate dielectric materials that have been examined during the past few years due to its relatively high resistivity, dielectric constant (16-45)[1,2], thermal stability and it compatibility with n+ polysilicon as the gate electrode material[3].

Zhao et.al. recently showed that variations in the crucial dielectric constant of HfO_2 are crystal phase dependent[4] Hence the structure of the crystal and electronic structure of HfO_2 thin films must be studied and correlated with their physical and electrical properties. Accordingly we have employed XANES and EXAFS to study 30 Å –750 Å HfO_2 films deposited on 11 Å SiO_xN_y/Si(100) by CVD.[5]. XAS measurements have been performed in the electron yield and fluorescence modes on the NSLS beam line X-18B.

Our preliminary results on the Hf $L_{2,3}$-edges in in these films system indicate that the 5d related white line (WL) are narrower in energy and weighted to lower energy relative to the bulk oxide. This is consistent with a smaller crystal field splitting and/or narrower 5d-band widths in the films. In addition the XAS fine structure above the Hf-L_3 edge evidence a slight increase in the average first shell Hf-O bond length in the thin films compared to bulk material. It is worth noting that the absence of the subtler fine structure features suggests a more disordered higher shell structure in the thin film.

Our XAS measurements and analysis on these and newly fabricated films are on going in conjunction with physical oroperty, electron spectroscopy and first principles band structure.

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